

chain nodes :

1 2 3 4 12 13

ring nodes :

5 6 7 8 9 10 15 16 17 18 19 20

chain bonds :

1-12 1-2 2-3 2-4 3-13 3-16 5-19

ring bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 2-3 2-4 3-16

exact bonds :

1-12 3-13 5-19

normalized bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

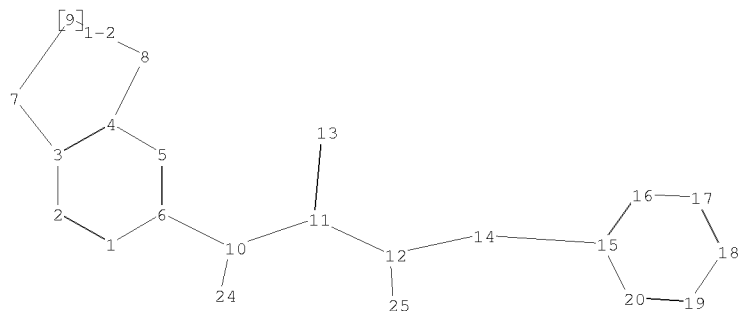
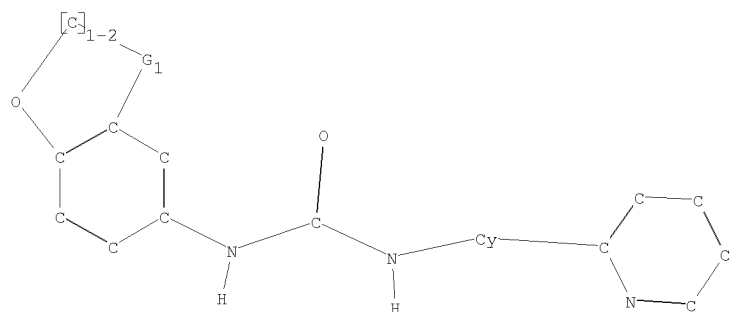
containing 15 :

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS  
13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom



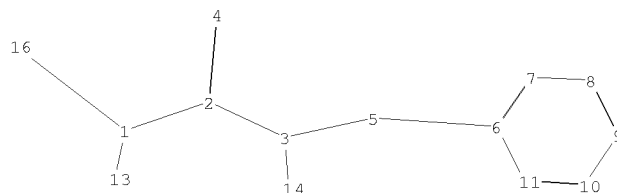
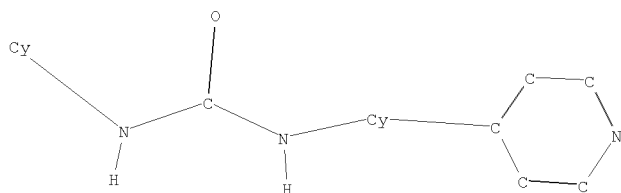
```

chain nodes :
  10 11 12 13 14 24 25
ring nodes :
  1 2 3 4 5 6 7 8 9 15 16 17 18 19 20
chain bonds :
  6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15
ring bonds :
  1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds :
  3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15
normalized bonds :
  1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems :
  containing 1 : 15 :
  
```

G1:C,O

```

Match level :
  1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS
  12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS
  25:CLASS
Generic attributes :
  14:
  Saturation : Unsaturated
  Number of Carbon Atoms : less than 7
  Number of Hetero Atoms : Exactly 1
  
```



chain nodes :

1 2 3 4 5 13 14 16

ring nodes :

6 7 8 9 10 11

chain bonds :

1-13 1-2 1-16 2-3 2-4 3-5 3-14 5-6

ring bonds :

6-11 6-7 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-16 2-3 2-4 3-5 5-6

exact bonds :

1-13 3-14

normalized bonds :

6-11 6-7 7-8 8-9 9-10 10-11

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

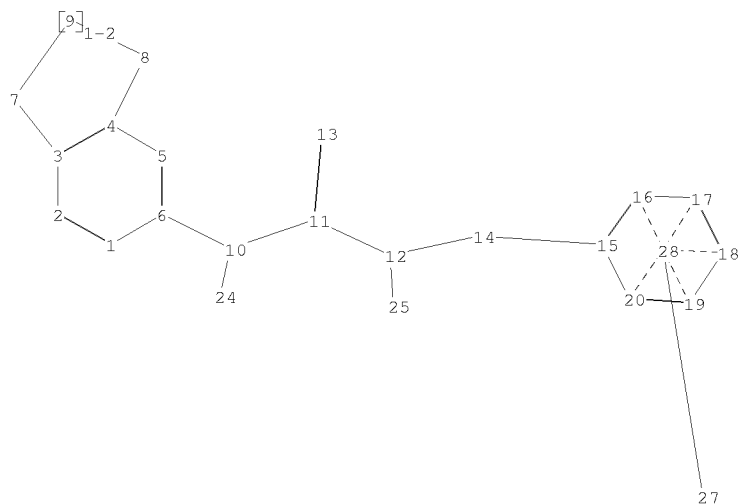
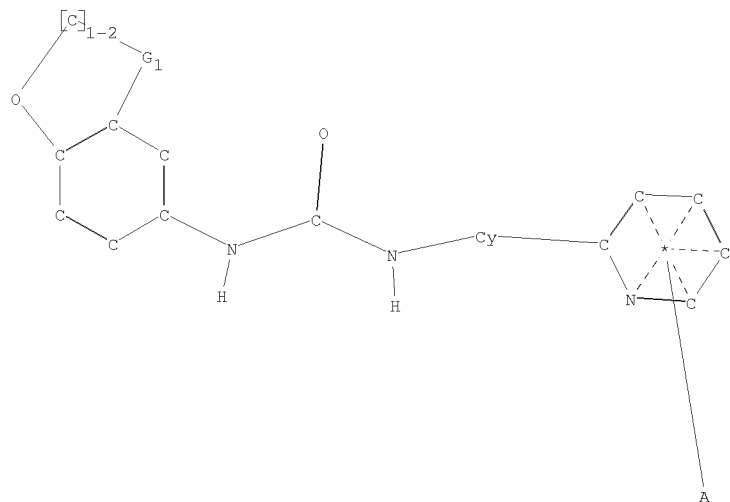
13:CLASS 14:CLASS 16:Atom

Generic attributes :

5:

Saturation : Unsaturated

Number of Hetero Atoms : Exactly 1



```

chain nodes :
  10 11 12 13 14 24 25 27
ring nodes :
  1 2 3 4 5 6 7 8 9 15 16 17 18 19 20
chain bonds :
  6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15
ring bonds :
  1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds :
  3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15
normalized bonds :
  1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems :
  containing 1 : 15 :

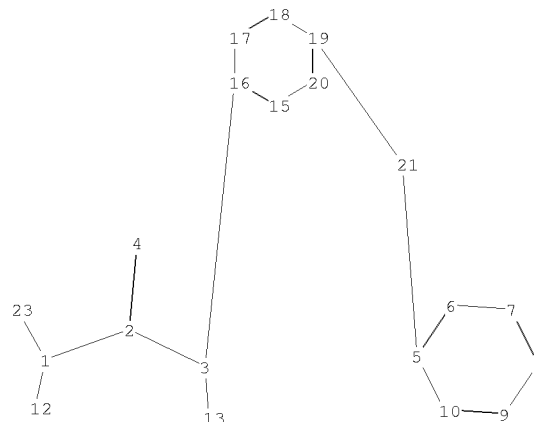
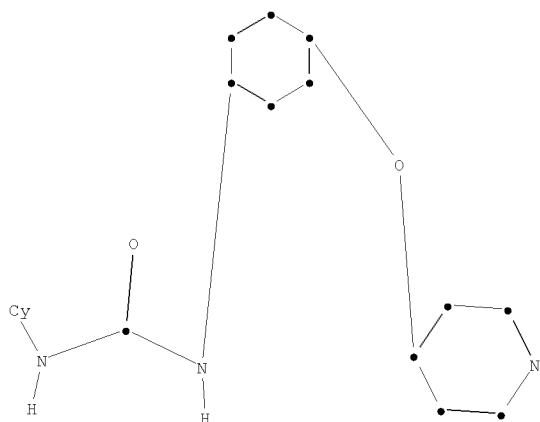
```

G1:C,O

```

Match level :
  1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS
  12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS
  25:CLASS 27:CLASS 28:CLASS
Generic attributes :
  14:
  Saturation : Unsaturated
  Number of Carbon Atoms : less than 7
  Number of Hetero Atoms : Exactly 1

```



chain nodes :

1 2 3 4 12 13 21 23

ring nodes :

5 6 7 8 9 10 15 16 17 18 19 20

chain bonds :

1-12 1-2 1-23 2-3 2-4 3-13 3-16 5-21 19-21

ring bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 1-23 2-3 2-4 3-16 5-21 19-21

exact bonds :

1-12 3-13

normalized bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 15 :

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level :

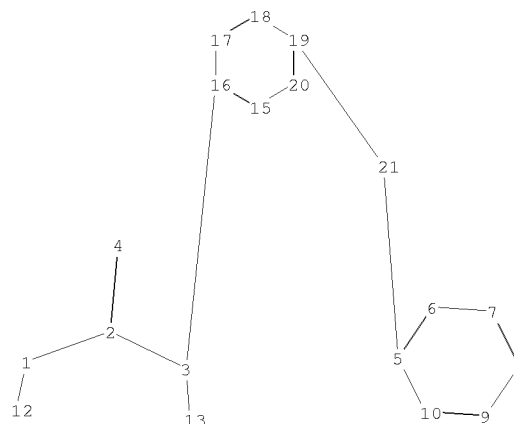
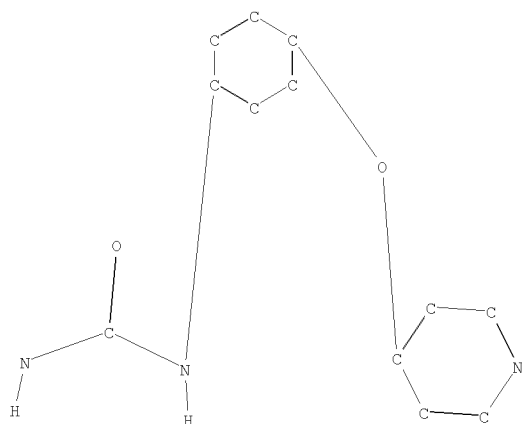
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS  
13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 23:Atom

Generic attributes :

23:

Number of Carbon Atoms : 7 or more

Type of Ring System : Polycyclic



chain nodes :

1 2 3 4 12 13 21

ring nodes :

5 6 7 8 9 10 15 16 17 18 19 20

chain bonds :

1-12 1-2 2-3 2-4 3-13 3-16 5-21 19-21

ring bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 2-3 2-4 3-16 5-21 19-21

exact bonds :

1-12 3-13

normalized bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

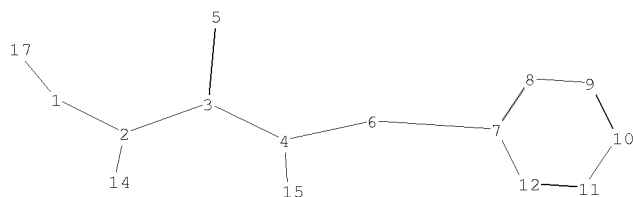
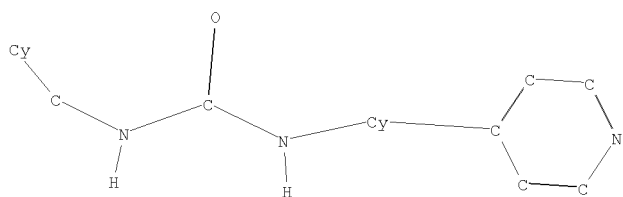
containing 15 :

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS  
13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS



```

chain nodes :
  1  2  3  4  5  6 14 15 17
ring nodes :
  7  8  9 10 11 12
chain bonds :
  1-2 1-17 2-3 2-14 3-4 3-5 4-6 4-15 6-7
ring bonds :
  7-12 7-8 8-9 9-10 10-11 11-12
exact/norm bonds :
  1-2 1-17 2-3 3-4 3-5 4-6 6-7
exact bonds :
  2-14 4-15
normalized bonds :
  7-12 7-8 8-9 9-10 10-11 11-12

```

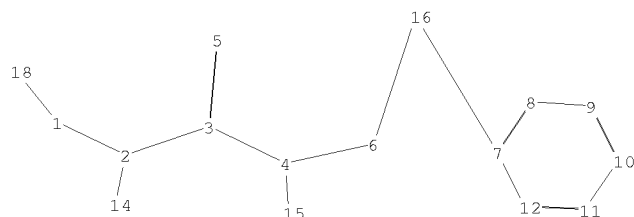
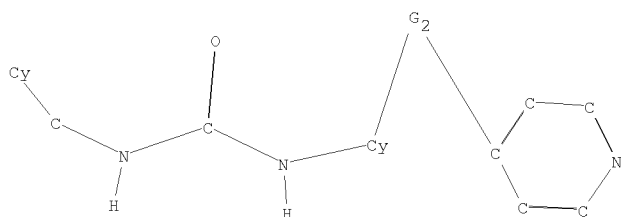
G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

```

Match level :
  1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
 12:Atom 14:CLASS 15:CLASS 17:Atom
Generic attributes :
6:
Saturation           : Unsaturated
Number of Hetero Atoms : Exactly 1

```



```

chain nodes :
  1  2  3  4  5  6 14 15 16 18
ring nodes :
  7  8  9 10 11 12
chain bonds :
  1-2 1-18 2-3 2-14 3-4 3-5 4-6 4-15 6-16 7-16
ring bonds :
  7-12 7-8 8-9 9-10 10-11 11-12
exact/norm bonds :
  1-2 1-18 2-3 3-4 3-5 4-6 6-16 7-16
exact bonds :
  2-14 4-15
normalized bonds :
  7-12 7-8 8-9 9-10 10-11 11-12

```

G1:C,O

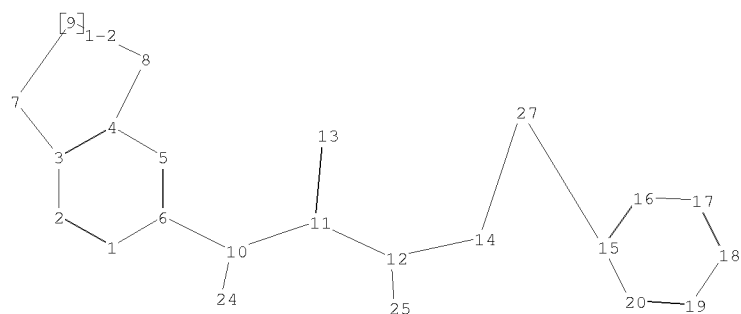
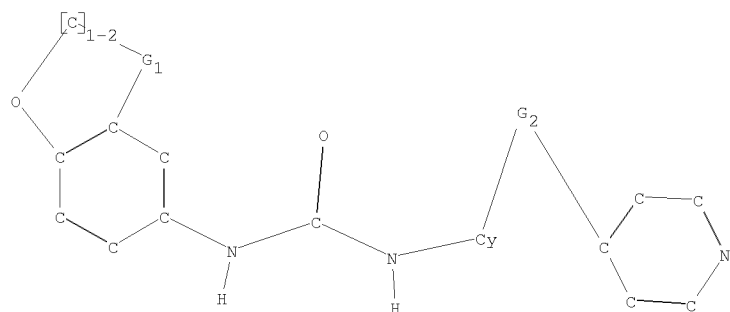
G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

```

Match level :
  1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
 12:Atom 14:CLASS 15:CLASS 16:CLASS 18:Atom
Generic attributes :
  6:
  Saturation           : Unsaturated
  Number of Hetero Atoms : Exactly 1

```





```

chain nodes :
  10 11 12 13 14 24 25 27
ring nodes :
  1 2 3 4 5 6 7 8 9 15 16 17 18 19 20
chain bonds :
  6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-27 15-27
ring bonds :
  1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-20 15-16 16-17 17-18 18-19 19-20
exact/norm bonds :
  3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-27 15-27
normalized bonds :
  1-2 1-6 2-3 5-6 15-20 15-16 16-17 17-18 18-19 19-20
isolated ring systems :
  containing 1 : 15 :

```

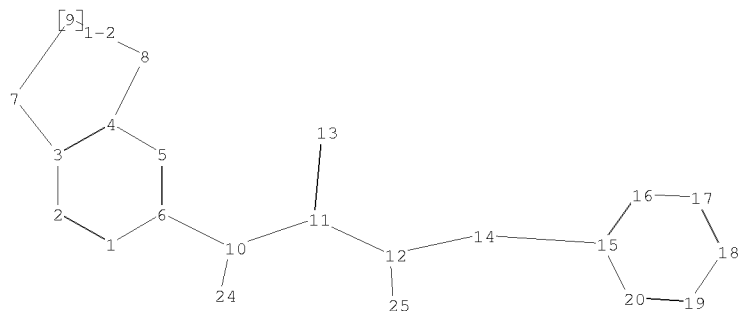
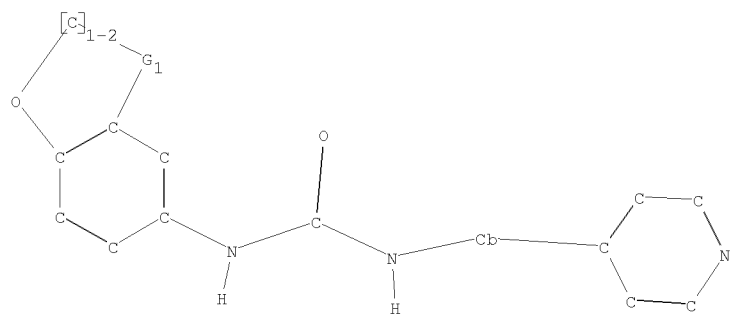
G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

```

Match level :
  1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS
  12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS
  25:CLASS 27:CLASS
Generic attributes :
  14:
  Saturation : Unsaturated
  Number of Hetero Atoms : Exactly 1

```



```

chain nodes :
  10 11 12 13 14 24 25
ring nodes :
  1 2 3 4 5 6 7 8 9 15 16 17 18 19 20
chain bonds :
  6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15
ring bonds :
  1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds :
  3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15
normalized bonds :
  1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems :
  containing 1 : 15 :

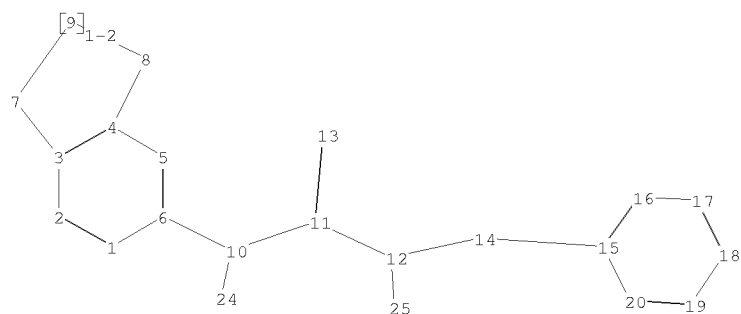
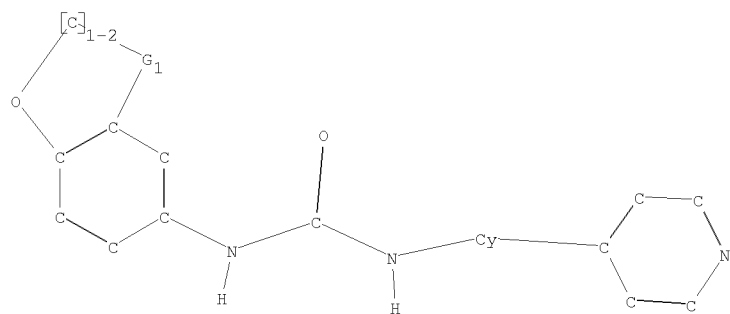
```

G1:C,O

```

Match level :
  1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS
  12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS
  25:CLASS

```



chain nodes :

10 11 12 13 14 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 15 16 17 18 19 20

chain bonds :

6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15

ring bonds :

1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15

normalized bonds :

1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 1 : 15 :

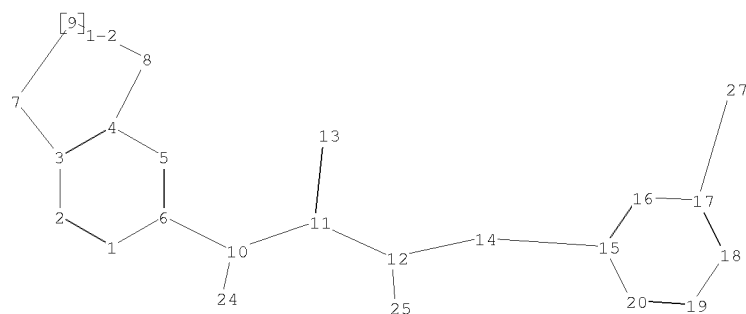
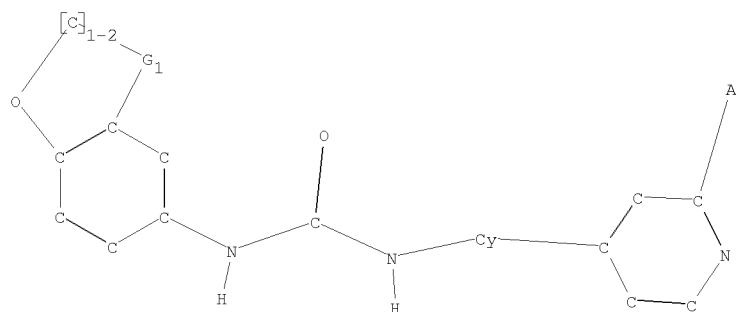
G1:C,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS  
12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS  
25:CLASS

Generic attributes :

14:  
Saturation : Unsaturated  
Number of Carbon Atoms : less than 7  
Number of Hetero Atoms : Exactly 1



chain nodes :

10 11 12 13 14 24 25 27

ring nodes :

1 2 3 4 5 6 7 8 9 15 16 17 18 19 20

chain bonds :

6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15 17-27

ring bonds :

1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15 17-27

normalized bonds :

1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 1 : 15 :

G1:C,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS  
12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS  
25:CLASS 27:CLASS

Generic attributes :

14:  
Saturation : Unsaturated  
Number of Carbon Atoms : less than 7  
Number of Hetero Atoms : Exactly 1